

# *Contents*

<b>1 INTRODUCTION</b>	<b>1</b>
1.1 Terminology 1	
1.1.1 Numerical and Symbolic Calculation, 1	
1.1.2 Numerical Methods and Algorithms, 4	
1.1.3 Numerical Methods and Numerical Analysis, 5	
1.2 MATLAB Overview 6	
1.3 Organization of the Book 7	
1.3.1 MATLAB Basics, 8	
1.3.2 Numerical Techniques, 8	
1.3.3 Cross-referencing of MATLAB Programs, 10	
1.4 Rating System for Exercises 10	
 <b>Part 1 MATLAB Basics</b>	 <b>13</b>
<b>2 INTERACTIVE COMPUTING WITH MATLAB</b>	<b>15</b>
2.1 Running MATLAB 15	

- 2.1.1 MATLAB as an Expression Evaluator, 18
- 2.1.2 MATLAB Variables, 20
- 2.1.3 Built-in Variables and Functions, 21
- 2.1.4 Functions and Commands, 22
- 2.1.5 On-line Help, 23
- 2.2 Matrices and Vectors 24
  - 2.2.1 Creating Matrices, 26
  - 2.2.2 Subscript Notation for Matrix Elements, 31
  - 2.2.3 Colon Notation, 33
  - 2.2.4 Deleting Elements from Vectors and Matrices, 35
  - 2.2.5 Mathematical Operations with Matrices, 36
  - 2.2.6 Reshaping Matrices, 42
- 2.3 Additional Types of Variables 45
  - 2.3.1 Complex Numbers, 45
  - 2.3.2 Strings, 48
  - 2.3.3 Polynomials, 51
- 2.4 Managing the Interactive Environment 52
  - 2.4.1 The MATLAB Workspace, 52
  - 2.4.2 Working with Data from External Files, 53
- 2.5 Plotting in MATLAB 63
  - 2.5.1 Line Plots, 63
  - 2.5.2 Annotating Plots, 66
  - 2.5.3 Subplots, 68
  - 2.5.4 Surface Plots, 69
  - 2.5.5 Contour Plots, 74
- 2.6 Summary 77

### **3 MATLAB PROGRAMMING**

**85**

- 3.1 Script m-Files 86
  - 3.1.1 Creating m-Files, 88
  - 3.1.2 Script Side Effects, 91
  - 3.1.3 Comment Statements, 93
- 3.2 Function m-Files 93
  - 3.2.1 Function Syntax, 94
  - 3.2.2 Input and Output Parameters, 94
  - 3.2.3 Primary and Secondary Functions, 98
- 3.3 Input and Output 100
  - 3.3.1 Prompting for User Input, 100
  - 3.3.2 Text Output, 101
- 3.4 Flow Control 105
  - 3.4.1 Relational Operators, 105

- 3.4.2 Operator Precedence, 107
- 3.4.3 `if ... else ...`, 108
- 3.4.4 Case Selection with `switch` Structure, 109
- 3.4.5 `for` Loops, 110
- 3.4.6 `while` loops, 114
- 3.4.7 The `break` Command, 115
- 3.4.8 The `return` Command, 117
- 3.5 Vectorization 118
  - 3.5.1 Using Vector Operations instead of Loops, 119
  - 3.5.2 Preallocating Memory for Vectors and Matrices, 120
  - 3.5.3 Vectorized Indexing and Logical Functions, 121
- 3.6 Deus ex Machina 128
  - 3.6.1 Variable Number of Input and Output Parameters, 129
  - 3.6.2 Global Variables, 133
  - 3.6.3 The `feval` Function, 134
  - 3.6.4 Inline Function Objects, 137
- 3.7 Summary 139

## **4 ORGANIZING AND DEBUGGING MATLAB PROGRAMS 151**

- 4.1 Organizing and Documenting m-files 152
  - 4.1.1 Use of a Consistent Style, 153
  - 4.1.2 Visual Blocking and Whitespace, 154
  - 4.1.3 Meaningful Variable Names, 155
  - 4.1.4 Documentation, 156
- 4.2 Organizing a Numerical Solution 159
  - 4.2.1 Stepwise Refinement, 160
  - 4.2.2 Implementation: One Program, Multiple m-files, 162
  - 4.2.3 Testing, 169
- 4.3 Debugging 173
  - 4.3.1 Defensive Programming, 174
  - 4.3.2 Debugging Tools, 176
- 4.4 Summary 180

## **Part 2 Numerical Techniques 185**

### **5 UNAVOIDABLE ERRORS IN COMPUTING 187**

- 5.1 Digital Representation of Numbers 191
  - 5.1.1 Bits, Bytes, and Words, 191
  - 5.1.2 Integers, 192
  - 5.1.3 Floating-point Numbers, 193

- 5.1.4 Numerical versus Symbolic Calculations, 201
- 5.2 Finite Precision Arithmetic 202
  - 5.2.1 Machine Precision, 209
  - 5.2.2 Implications for Routine Calculations, 210
  - 5.2.3 Measuring Errors, 211
  - 5.2.4 Convergence of Iterative Sequences, 213
  - 5.2.5 Relative and Absolute Convergence Criteria, 216
- 5.3 Truncation Error of Algorithms 217
  - 5.3.1 Taylor Series, 221
  - 5.3.2 Order Notation, 223
- 5.4 Summary 232

## **6 FINDING THE ROOTS OF $f(x) = 0$**

**240**

- 6.1 Preliminaries 243
  - 6.1.1 General Considerations, 243
  - 6.1.2 The Basic Root-finding Procedure, 244
  - 6.1.3 Bracketing, 245
- 6.2 Fixed-point Iteration 250
  - 6.2.1 Convergence of Fixed-point Iteration, 253
- 6.3 Bisection 253
  - 6.3.1 Analysis of the Bisection Method, 256
  - 6.3.2 Convergence Criteria, 257
  - 6.3.3 A General Implementation of Bisection, 259
- 6.4 Newton's Method 261
  - 6.4.1 Convergence of Newton's Method, 264
  - 6.4.2 A General Implementation of Newton's Method, 265
- 6.5 The Secant Method 268
- 6.6 Hybrid Methods 273
  - 6.6.1 The `fzero` Function, 273
- 6.7 Roots of Polynomials 279
  - 6.7.1 The `roots` Function, 280
- 6.8 Summary 283

## **7 A REVIEW OF LINEAR ALGEBRA**

**293**

- 7.1 Vectors 294
  - 7.1.1 Vector Operations, 296
  - 7.1.2 Vector Norms, 301
  - 7.1.3 Orthogonal Vectors, 308
- 7.2 Matrices 309
  - 7.2.1 The Rows and Columns of a Matrix Are Vectors, 309

- 7.2.2 Matrix Operations, 310
- 7.2.3 Operation Counts for Matrix and Vector Operations, 331
- 7.2.4 Matrix Norms, 333
- 7.3 Mathematical Properties of Vectors and Matrices 334
  - 7.3.1 Linear Independence, 335
  - 7.3.2 Vector Spaces, 336
  - 7.3.3 Subspaces Associated with Matrices, 339
  - 7.3.4 Matrix Rank, 341
  - 7.3.5 Matrix Determinant, 342
- 7.4 Special Matrices 346
  - 7.4.1 Diagonal Matrices, 346
  - 7.4.2 The Identity Matrix, 347
  - 7.4.3 The Matrix Inverse, 348
  - 7.4.4 Symmetric Matrices, 349
  - 7.4.5 Tridiagonal Matrices, 349
  - 7.4.6 Positive Definite Matrices, 351
  - 7.4.7 Orthogonal Matrices, 351
  - 7.4.8 Permutation Matrices, 352
- 7.5 Summary 353

## **8 SOLVING SYSTEMS OF EQUATIONS**

**363**

- 8.1 Basic Concepts 365
  - 8.1.1 Matrix Formulation, 365
  - 8.1.2 Requirements for a Solution, 369
- 8.2 Gaussian Elimination 379
  - 8.2.1 Solving Diagonal Systems, 379
  - 8.2.2 Solving Triangular Systems, 380
  - 8.2.3 Gaussian Elimination without Pivoting, 382
  - 8.2.4 Gaussian Elimination with Pivoting, 387
  - 8.2.5 Solving Systems with the Backslash Operator, 396
- 8.3 Limitations on Numerical Solutions to  $Ax = b$  398
  - 8.3.1 Computational Work, 398
  - 8.3.2 Sensitivity to Inputs, 399
  - 8.3.3 Computational Stability, 405
  - 8.3.4 The Residual, 407
  - 8.3.5 Rules of Thumb, 407
  - 8.3.6 Computing  $\kappa(A)$ , 408
- 8.4 Factorization Methods 410
  - 8.4.1 LU Factorization, 410
  - 8.4.2 Cholesky Factorization, 422
  - 8.4.3 The Backslash Operator Reconsidered, 426

- 8.5 Nonlinear Systems of Equations 427
  - 8.5.1 Iterative Methods for Nonlinear Systems, 427
  - 8.5.2 Successive Substitution, 429
  - 8.5.3 Newton's Method, 432
- 8.6 Summary 443

## **9 LEAST-SQUARES FITTING OF A CURVE TO DATA 455**

- 9.1 Fitting a Line to Data 458
  - 9.1.1 Minimizing the Residual, 460
  - 9.1.2 An Overdetermined System of Equations, 461
  - 9.1.3 Implementation of Line Fitting, 463
  - 9.1.4 The  $R^2$  Statistic, 464
  - 9.1.5 Fitting Lines to Apparently Nonlinear Functions, 468
  - 9.1.6 Summary of Fitting Data to a Line, 472
- 9.2 Least-Squares Fit to a Linear Combination of Functions 473
  - 9.2.1 Basis Functions, 474
  - 9.2.2 Least-Squares Fit via Solution to the Normal Equations, 475
  - 9.2.3 Least-Squares Approximation with QR Factorization, 485
  - 9.2.4 Polynomial Curve Fitting, 495
- 9.3 Multivariate Linear Least-Squares Fitting 500
- 9.4 Summary 508

## **10 INTERPOLATION 521**

- 10.1 Basic Ideas 524
  - 10.1.1 Interpolation versus Curve Fitting, 525
  - 10.1.2 Interpolation and Extrapolation, 525
- 10.2 Interpolating Polynomials of Arbitrary Degree 527
  - 10.2.1 Polynomial Interpolation with a Monomial Basis, 527
  - 10.2.2 Polynomial Interpolation with a Lagrange Basis, 532
  - 10.2.3 Polynomial Interpolation with a Newton Basis, 538
  - 10.2.4 Polynomial Wiggle, 552
- 10.3 Piecewise Polynomial Interpolation 554
  - 10.3.1 Piecewise-Linear Interpolation, 556
  - 10.3.2 Searching for Support Points, 557
  - 10.3.3 The `interp` Function, 559
  - 10.3.4 Piecewise-Cubic Hermite Interpolation, 560
  - 10.3.5 Cubic Spline Interpolation, 568
- 10.4 MATLAB's Built in Interpolation Functions 583
  - 10.4.1 One-dimensional Interpolation with `interp1` and `spline`, 584
- 10.5 Summary 586

## **11 NUMERICAL INTEGRATION**

**597**

- 11.1 Basic Ideas and Nomenclature 600
  - 11.1.1 Symbolic versus Numerical Integration, 602
- 11.2 Newton–Cotes Rules 603
  - 11.2.1 Trapezoid Rule, 603
  - 11.2.2 Simpson’s Rule, 612
  - 11.2.3 Catalog of Newton–Cotes Rules, 616
- 11.3 Gaussian Quadrature 620
  - 11.3.1 Theoretical Basis, 622
  - 11.3.2 The Basic Rule for Gauss–Legendre Quadrature, 626
  - 11.3.3 Table Lookup for Nodes and Weights, 628
  - 11.3.4 Computing the Nodes and Weights, 629
  - 11.3.5 Composite Rule for Gauss–Legendre Quadrature, 634
- 11.4 Adaptive Quadrature 644
  - 11.4.1 Adaptive Integration Based on Simpson’s Rule, 646
  - 11.4.2 Built-in quad and quad8 Functions, 654
  - 11.4.3 New quad and quad1 Functions, 659
- 11.5 Improper Integrals and Other Complications 660
  - 11.5.1 Integrals with Infinite Limits, 660
- 11.6 Summary 666

## **12 NUMERICAL INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS**

**674**

- 12.1 Basic Ideas and Nomenclature 676
  - 12.1.1 Ordinary Differential Equations, 676
  - 12.1.2 Overview of Numerical Solution Strategy, 679
- 12.2 Euler’s Method 681
  - 12.2.1 Implementation of Euler’s Method, 683
  - 12.2.2 Analysis of Euler’s Method, 686
  - 12.2.3 Generalization: One-Step Methods, 691
  - 12.2.4 Summary of §12.2, 692
- 12.3 Higher Order One-step Methods 692
  - 12.3.1 Midpoint Method, 693
  - 12.3.2 Heun’s Method, 696
  - 12.3.3 Fourth-order Runge–Kutta Method, 697
- 12.4 Adaptive Step-size Algorithms 700
  - 12.4.1 The ode23 and ode45 Routines, 701
- 12.5 Coupled ODEs 710
  - 12.5.1 The RK-4 Algorithm for Coupled ODEs, 713
  - 12.5.2 Higher Order Differential Equations, 720

12.6	Additional Topics	724
12.7	Summary	725
<b>BIBLIOGRAPHY</b>		<b>735</b>
<b>APPENDIX A EIGENVALUES AND EIGENSYSTEMS</b>		<b>741</b>
A.1	Eigenvectors Map onto Themselves	742
A.2	Mathematical Preliminaries	745
A.2.1	Characteristic Polynomial,	745
A.2.2	Companion Matrix,	746
A.2.3	Eigenfacts,	746
A.3	The Power Method	748
A.3.1	Power Iterations,	749
A.3.2	Inverse-Power Iterations,	751
A.4	Built-in Functions for Eigenvalue Computation	753
A.4.1	The eig Function,	753
A.4.2	The eigs Function,	755
A.5	Singular Value Decomposition	755
A.5.1	The svd Function,	756
<b>APPENDIX B SPARSE MATRICES</b>		<b>757</b>
B.1	Storage and Flop Savings	758
B.2	MATLAB Sparse Matrix Format	758
B.2.1	Creating Sparse Matrices,	759
B.2.2	Operations on Sparse Matrices,	766
<b>MATLAB TOOLBOX FUNCTIONS</b>		<b>769</b>
<b>LISTINGS FOR NMM TOOLBOX m-FILES</b>		<b>773</b>
<b>SUBJECT INDEX</b>		<b>775</b>